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Conformational analysis of 2-substituted nitroethenes

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Abstract

Experimental and theoretical conformational analysis of polyfunctional 2-substituted nitroethenes was carried out by the method of dipole moments and density functional theory calculations. It was established that the nitro and ester (or trichloromethyl) groups are trans-arranged in the molecules of 2-trichloromethyl-(ethoxycarbonyl)-1-nitro- and 1-bromo-1-nitroethenes, i.e., nitroalkenes have E-configuration, their bromo-containing analogues have Z-configuration, and s-cis-orientation of the C=C and C=O double bonds is preferred for nitroacrylates. 2,3-Dibromo-3-nitroacrylates have untrivial Z-configuration in solution. © 2010 Springer Science+Business Media, LLC.

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Keywords

Conformational analysis, DFT calculations, Dipole moments, Nitroethenes